



TITLE:

Studies on the Molecular Structures of BHC  
and its Related Compounds. (II) : On the  
Molecular Structure of  $\gamma$ -  
Monochlorobenzene Hexachloride

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and the physical properties were determined.

Then we tested the insecticidal activities of the following materials against houseflies (*Musca domestica* L.): Four fractions of Reaction A (F-1~4);  $\alpha$ -heptachlorocyclohexane (mp. 153-4°);  $\gamma$ -heptachlorocyclohexane (84-5°); *o*-octachlorocyclohexane (149°);  $\beta$ -*p*-octachlorocyclohexane (262°);  $\gamma$ -BHC.

The modified turn table method was adopted and the testing results are shown in the Table.

Toxicity of Chlorinated Compounds of BHC against Houseflies.  
(Kill in 24 hours, per cent)

mg/cc	$\gamma$ -BHC	F-1	F-2	F-3	F-4	$\alpha$ -hepta	$\gamma$ -hepta	<i>o</i> -octa	$\beta$ - <i>p</i> -octa
0.00025	34.3	—	—	—	—	—	—	—	—
0.0005	41.8	—	—	—	—	—	—	—	—
0.001	51.1	—	—	—	—	—	—	—	—
0.002	62.5	—	—	—	—	—	—	—	—
0.125	—	45.5	49.5	38.9	21.8	62.7	48.1	75.2	22.5
0.25	—	55.3	59.7	50.2	30.9	74.8	59.2	78.5	44.6
0.5	—	68.0	72.9	61.8	37.5	83.8	64.0	84.3	61.9
1.0	—	82.4	86.1	72.9	42.6	90.7	72.6	88.0	—

In these tests only  $\gamma$ -BHC is found very effective while chlorinated products of  $\gamma$ -BHC and other highly chlorinated compounds all ineffective. So in the technical preparation it is preferable to remove  $\gamma$ -BHC from the reaction system which might be produced from benzene and chlorine, as soon as possible in order to avoid further chlorination.

#### 74. Studies on the Molecular Structures of BHC and its Related Compounds. (II)

On the Molecular Structure of  $\gamma$ -Monochlorobenzene Hexachloride.

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In the previous reports (Oiwa, T., et al: *Botyu-Kagaku*, 14, 42 (1949); *ibid.*, 15, 32 (1950)) we published the details of our investigations about the molecular structures of BHC and its related compounds. In this paper we report the molecular configuration of  $\gamma$ -monochlorobenzene hexachloride (mp. 85-86°).

Two grams of  $\gamma$ -monochlorobenzene hexachloride were chlorinated in the 150 grams of carbon tetrachloride containing 6 grams of chlorine under the light for 1 hour. After the removal of the solvent 2.16 grams of slightly yellowish oily matter was obtained. Then from this matter 0.15 gram of colorless crystals

(mp. 149°) were isolated by partition chromatography and recrystallization, and it was found that these crystals were undoubtedly the same as o-dichlorobenzene hexachloride (mp. 149.5–150°) from the results of mixed melting point, chlorine content, half wave potential and alkaline decomposition.

It was already been discussed that the structures of cyclohexane and its chlorinated derivatives had chair form. And the molecular configuration of o-dichlorobenzene hexachloride has been determined to be the chlorine configuration  $(\widehat{pe} \ e \ e \ e \ e \ \widehat{pe})$ . As we can expect only two chlorine configurations of monochlorobenzene hexachloride which will be chlorinated to o-dichlorobenzene hexachloride and one of which  $(\widehat{pe} \ e \ e \ e \ e \ e)$  was already determined as  $\alpha$ -monochlorobenzene hexachloride (mp. 153–154°), so the other chlorine configuration  $(\widehat{pe} \ e \ e \ e \ e \ p)$  would be  $\gamma$ -monochlorobenzene hexachloride.

Although in the previous report we assumed the molecular configuration of  $\gamma$ -monochlorobenzene hexachloride from the polarographic studies of the chlorinated substance of  $\alpha$ - and  $\gamma$ -BHC, we amend it as described above.